

2-Isopropyl-6-methyl-4-pyrimidone
2814-20-2 | DTXSID1027502

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.54e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.21e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Barban</div> <div>Measured: 3.75e-05</div> <div>Predicted: 1.55e-06</div>	<div>Image not found</div> <div>N-Ethylaniline</div> <div>Measured: 3.57e-03</div> <div>Predicted: 1.48e-01</div>	<div>Image not found</div> <div>Phenylacetic acid</div> <div>Measured: 2.00e-04</div> <div>Predicted: 8.09e-04</div>
<div>Image not found</div> <div>2-Ethylphenol</div> <div>Measured: 5.93e-01</div> <div>Predicted: 6.07e-02</div>	<div>Image not found</div> <div>Ethyl propionate</div> <div>Measured: 1.60e-03</div> <div>Predicted: 32.4</div>	